INTERFACE DISCONTINUITY FACTORS IN THE MODAL EIGENSPACE OF THE MULTIGROUP DIFFUSION MATRIX

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ABSTRACT

Interface discontinuity factors based on the Generalized Equivalence Theory are commonly used in nodal homogenized diffusion calculations so that diffusion average values approximate heterogeneous higher order solutions. In this paper, an additional form of interface correction factors is presented in the frame of the Analytic Coarse Mesh Finite Difference Method (ACMFD), based on a correction of the modal fluxes instead of the physical fluxes.

In the ACMFD formulation, implemented in COBAYA3 code, the coupled multigroup diffusion equations inside a homogenized region are reduced to a set of uncoupled modal equations through diagonalization of the multigroup diffusion matrix. Then, physical fluxes are transformed into modal fluxes in the eigenspace of the diffusion matrix. It is possible to introduce interface flux discontinuity jumps as the difference of heterogeneous and homogeneous modal fluxes instead of introducing interface discontinuity factors as the ratio of heterogeneous and homogeneous physical fluxes. The formulation in the modal space has been implemented in COBAYA3 code and assessed by comparison with solutions using classical interface discontinuity factors in the physical space.

Key Words: Interface discontinuity factor, interface discontinuity jumps, eigenvector modal space.

1. INTRODUCTION

The accuracy of nodal homogenized diffusion calculations lies in an efficient and accurate multi-group nodal diffusion code as well as in the determination of adequate multigroup homogenized parameters to be used by the core code. In order that the calculation of the homogenized system yields average values close to the ones obtained in a heterogeneous detailed and higher order problem, correction factors must be introduced. These factors account for all the approximations made in the nodal diffusion calculation, namely homogenization, condensation, transport and meshing effects.

Interface discontinuity factors (IDF) based on the Generalized Equivalence Theory (GET) [1,2] are the most common option to correct these compendium of errors, and are defined as the ratio of the face-averaged heterogeneous and homogeneous fluxes. Through GET, the flux distribution is modified from that obtained in homogenized regions, making nodal reaction rates and inter-nodal leakage to be equivalent to those of the heterogeneous reference problem.

Calculating accurate IDF requires the knowledge of the heterogeneous neutron flux distribution, and in general, this flux will not be known for the configuration being computed. Then, it is common practice to approximate it with the neutron flux from single assembly calculations with zero-current boundary conditions. However, the boundary conditions of any node in the true core environment will differ from zero-net-current, so that the actual discontinuity factors will differ from those computed in an infinite lattice. This will be particularly noticeable near the core periphery or next to control elements.

An alternative to generate accurate IDF is to calculate reference values using zero-net-current boundary conditions for each homogenized region and to synthesize afterwards their dependencies on the main neighborhood variables. In such a way the IDF could be better approximated during nodal diffusion calculations by correcting the reference values using the actual nodal boundary conditions. A parameterization of the IDF depending on neighborhood for pin-by-pin diffusion calculations is proposed in another paper presented to this conference [3] and similar work is in progress at nodal level.

This paper studies an additional definition of interface correction factors to be applied in the frame of the Analytic Coarse Mesh Finite Difference Method (ACMFD), based on a correction of the modal fluxes instead of the physical fluxes. In the ACMFD formulation, the coupled multigroup diffusion equations inside a homogenized region are reduced to a set of uncoupled modal equations through diagonalization of the multigroup diffusion matrix. Then, physical fluxes are transformed into modal fluxes in the eigenspace of the diffusion matrix. It is possible to introduce interface flux discontinuity jumps as the difference of heterogeneous and homogeneous modal fluxes instead of introducing interface discontinuity factors as the ratio of heterogeneous and homogeneous physical fluxes.

The present work is concerned with investigating the adequacy of interface flux discontinuity jumps in the modal space for nodal diffusion calculations. First, the correction factors computed for single-assembly calculations are analyzed. Then, different color-set configurations are used in order to assess the effects of the leakage on the modal jumps. The methodology has been implemented in our in-house multi-group neutron diffusion code COBAYA3 [4,5] and verified by comparison with solutions using classical interface discontinuity factors in the physical space.

2. INTERFACE DISCONTINUITY FACTORS IN THE ANALYTIC COARSE MESH FINITE DIFFERENCE METHOD

For stand-alone nodal calculations, COBAYA3 code uses an analytic nodal diffusion solver called ANDES [4,5], based on the Analytic Coarse-Mesh Finite-Difference (ACMFD) method.

2.1. The Analytic Coarse Mesh Finite Difference Method (ACMFD)

When we try to solve the set of G multi-group diffusion equations inside a homogenized region, we find that they are coupled by fission and scattering terms. The equations can be expressed in vector form using bra-ket notation:

$$\nabla^2 \left|\phi(r)\right\rangle - A\left|\phi(r)\right\rangle = -D^{-1}\left|S(r)\right\rangle \tag{1}$$

Where A is called the multi-group diffusion matrix and includes absorption, fission and scattering terms. The external source distribution $\left|S\right\rangle$ includes the transverse leakage. The way to solve the coupled linear system is to diagonalize the matrix A which is non-singular so it can be written as follows:

$$A\left|u_m\right\rangle = \lambda_m \left|u_m\right\rangle \quad ; \quad R^{-1} = \left[u_m\right] \quad ; \quad A = R^{-1}\left[\lambda_m\right]_{diag} R \tag{2}$$

Where λ_m and u_m are respectively the eigenvalue and eigenvector for mode *m*. Thus, pre-multiplying equation (1) by matrix R of a base of eigenvectors and assuming that:

$$\left|\phi_g\right\rangle = R^{-1}\left|\psi_m\right\rangle \quad ; \quad \left|S_g\right\rangle = DR^{-1}\left|s_m\right\rangle \tag{3}$$

The G multigroup coupled equations (1) are reduced to another G uncoupled *modal* equations (4). Solutions for these equations are the *modal fluxes* which are related to the physical fluxes by a linear relation (3).

$$\nabla^2 \psi_m(r) - \lambda_m \psi_m(r) = -s_m(r) \quad , \quad m = 1 \ldots G \tag{4}$$

2.2. GET Interface Discontinuity Factors

GET interface discontinuity factors are defined as the ratio of the face-averaged heterogeneous flux to the face-averaged homogeneous flux per energy group. A GxG diagonal matrix of scalar factors in the physical space per nodal interface F_d is obtained:

$$\left|\phi_g^{het}(\mp\tfrac{H}{2})\right\rangle = F_d \left|\phi_g^{\hom}(\mp\tfrac{H}{2})\right\rangle = \begin{bmatrix} f_1 & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & f_G \end{bmatrix} \left|\phi_g^{\hom}(\mp\tfrac{H}{2})\right\rangle \tag{5}$$

- For a single assembly calculation with reflective boundary conditions, the homogeneous flux distribution profile would be flat, so the homogeneous interface fluxes would be equal to the node averaged ones. The corresponding factor is called Single Assembly Discontinuity Factor (SADF) and can be computed directly from the transport solution as the quotient of the interface and averaged fluxes:

$$J_g^{het} = 0 \Rightarrow \phi_s^{\text{hom}} = \bar{\phi}^{het} \Rightarrow f_{SADF} = \frac{\phi_s^{het}}{\bar{\phi}^{het}} \tag{6}$$

- If the fuel assembly is not in an infinite lattice but has non-zero current boundary conditions, IDFs will depend on the method used to obtain the homogeneous interface fluxes in the diffusion nodal calculation. In the ACMFD method implemented in ANDES, after solving the modal equations (4) and transforming the modal fluxes to the physical space, the homogeneous interface flux is computed as follows:

$$R\left|\phi_g^{\text{hom}}\right\rangle_{(\mp\frac{H}{2})} = C^f R\left|\bar{\phi}_g\right\rangle \pm \frac{H}{2} C^j R D_g^{-1}\left|J_g\right\rangle_{(\mp\frac{H}{2})} - \left|T\right\rangle_{(\mp\frac{H}{2})} \tag{7}$$

  Where vector T is related to transverse leakage and C^f and C^j are GxG matrices, so we can notice matrix relationships involving dependencies of the interface flux for each group on the values of all energy groups.

  In order to compute IDFs at the nodal level, the detailed transport calculation must provide per energy group: the node averaged fluxes, the interface averaged fluxes and currents (that allow also to compute the vector related to transverse leakage) and the multigroup diffusion matrix (which includes absorption, fission and scattering cross sections as well as diffusion coefficients).

  Once computed the IDF matrix, the relationship between interface currents, interface fluxes and node averaged fluxes in ANDES calculation is given by the following matrix-vector equation, where the heterogeneous fluxes (and not the homogeneous ones) are continuous across the boundaries:

$$RF_d^{-1}\left|\phi_g^{het}\right\rangle_{(\mp\frac{H}{2})} = C^f R\left|\bar{\phi}_g\right\rangle \pm \frac{H}{2} C^j R D_g^{-1}\left|J_g\right\rangle_{(\mp\frac{H}{2})} - \left|T\right\rangle_{(\mp\frac{H}{2})} \tag{8}$$

2.3. Interface Modal Jumps in the Eigenvector Modal Space

An additional form of the interface correction factor can be presented for the ACMFD formulation based on a correction of the modal fluxes instead of the physical ones. The actual heterogeneous physical fluxes at the node interfaces, calculated by a higher-order and detailed calculation, are first transformed to the modal space through the eigenvector matrix R using Eq. (3).

Once the homogeneous interface modal fluxes are computed following expression (7) but in the modal space, a correction can be introduced to force those homogeneous quantities to meet the values of the heterogeneous modal ones. That is, we introduce interface modal flux discontinuity jumps (MJ) or differences at each node interface per mode by:

$$R\left|\phi_g^{het}\right\rangle_{(\mp\frac{H}{2})} = \left|\psi_m^{het}\right\rangle_{(\mp\frac{H}{2})} \quad ; \quad \left|\psi_m^{het}\right\rangle_{(\mp\frac{H}{2})} = \left|\psi_m^{\hom}\right\rangle_{(\mp\frac{H}{2})} + \left|d_m\right\rangle_{(\mp\frac{H}{2})} \tag{9}$$

And when applying the change of base back to the physical space we find that the heterogeneous (continuous) physical group fluxes are related to the homogeneous (discontinuous) physical fluxes by an additive term (instead of a multiplicative one as in Eq. 5 for the IDF) which is a matrix-vector product that couples all the modal jumps for each energy group:

$$\left|\phi_g^{het}\right\rangle_{(\mp\frac{H}{2})} = \left|\phi_g^{\hom}\right\rangle_{(\mp\frac{H}{2})} + \left|MJ_d\right\rangle_{(\mp\frac{H}{2})} \quad ; \quad \left|MJ_d\right\rangle_{(\mp\frac{H}{2})} = R^{-1}\left|d_m\right\rangle_{(\mp\frac{H}{2})} \tag{10}$$

Where $\left|d_m\right\rangle$ is the vector of modal discontinuity jumps at the interface, defined by (9), which can be real or complex, since the modal fluxes are complex for the modes with complex eigenvalues; and $\left|MJ_d\right\rangle$ is the new real vector of physical flux discontinuity jumps at each node interface.

- In a single assembly calculation, modal jumps are computed as follows. First, eigenvalues and eigenvectors are calculated; the fundamental eigenvalue is zero since the node is critical as a B1 buckling search is performed, while transient eigenvalues can be real or complex and always have a positive and increasing real part, showing how the associated modal terms vanish much faster with the distance from the boundaries. If the assembly is considered to be homogeneous, the flux distribution profile will be flat ($\phi_{g\,(\mp\frac{H}{2})} = \overline{\phi}_g$); that is, the fundamental mode (*fm*) would be reached, and all transient modes (*tm*) would be zero:

$$\psi^{\hom}_{\mathrm{fm}\ (\mp\frac{H}{2})} = \overline{\psi}_{\mathrm{fm}} \quad \wedge \quad \psi^{\hom}_{\mathrm{tm}\ (\mp\frac{H}{2})} = 0 \tag{11}$$

  For a heterogeneous assembly, once calculated the heterogeneous interface modal flux, the jump for the fundamental mode is:

$$d_{fm(\mp\frac{H}{2})} = \psi^{het}_{fm\ (\mp\frac{H}{2})} - \overline{\psi}_{fm} \tag{12}$$

  And the jumps for the transient modes coincide with the values of the heterogeneous modal fluxes from the reference solution:

$$d_{tm(\mp\frac{H}{2})} = \psi^{het}_{tm\ (\mp\frac{H}{2})} \tag{13}$$

Since $\psi^{hom}_{tm\ (T\frac{H}{2})} = 0$ it is not possible to define a correction factor as the quotient of the interface modal heterogeneous and homogeneous fluxes, like in the physical space.

- If the fuel assembly is not in an infinite lattice, the homogeneous modal flux can be computed by (7); the heterogeneous modal flux from the detailed transport calculation and the modal jumps are obtained from (9).

3. PROBLEM DESCRIPTION

In order to evaluate the merits of this formulation, several transport calculations were performed for different single assembly and color-set configurations. Specifications were taken from a NURESIM benchmarking document [6]. All the transport calculations were performed with NEWT code from the SCALE6.0 code package [7], using the ENDF/B-5 library in 44 energy groups suitable for light water reactors. NEWT was chosen since it provides interface average fluxes and currents as required to compute the interface correction factors. Collapsing in 2, 4 and 8 energy groups was performed, allowing the analysis of the dependencies on the number of energy groups considered.

Interface correction factors were computed in both physical and modal spaces for the four different types of 17x17 assemblies with reflective boundary conditions represented in Fig. 1: an uranium-oxide fresh fuel assembly (UOX) with 4.2 $^{w}/_{o}$ enrichment, a rodded UOX fuel assembly at 37.5 GWd/t_{HM} (UOX-R), a UOX assembly with 12 Gd pins (Gd-UOX) and a mixed-oxide fuel assembly (MOX) with three different Pu enrichments (7.8%, 5.2% and 3.2%).

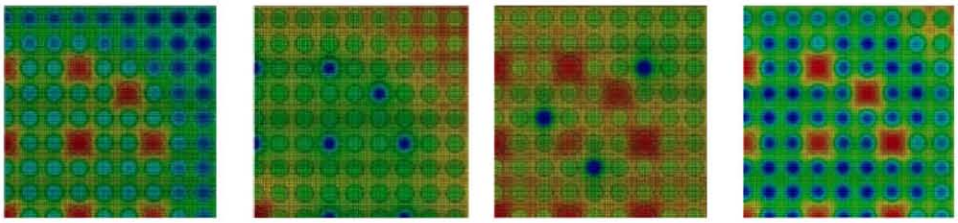

Figure 1. Representation of ¼ of the assembly considered: UOX, UOX with control rods, Gd-UOX and MOX.

In order to analyze how the interface correction factors (both IDF and MJ) change when actual node environment differs from reflective boundary conditions, a group of representative color-sets or clusters of quarters of fuel assemblies were chosen. Configurations in 1D and 2D, such as sketched in Fig. 2, were defined with reflective boundary conditions. Each fuel assembly was combined with every other fuel assembly types.

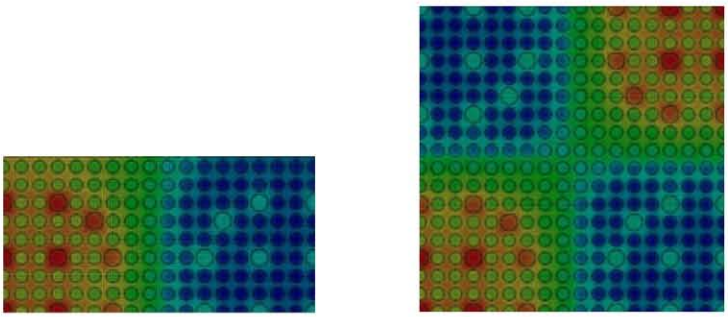

Figure 2. Clusters of two quarters of fuel assemblies with reflective boundary conditions: 1D color-set and 2D color-set configurations.

4. MODAL JUMPS ANALYSIS

4.1. Single Assembly Calculations

The lattice code NEWT was used to perform transport single assembly calculations with critical leakage. Interface discontinuity factors in physical space were directly obtained and modal jumps were computed with ANDES solver. Since the fluxes provided by NEWT had to be transformed into the modal space through diagonalization of the multigroup diffusion matrix ANDES was adapted to generate IDF and MJ in any number of energy groups.

Representations of the IDF in the energy range are made in Fig. 3 for the four types of fuel assemblies analyzed where a stronger correction is seen for the external interface of the fuel assembly and for thermal groups. It is worthy to mention that for few energy groups, all groups present a considerable degree of correction through the IDF and not only the thermal ones.

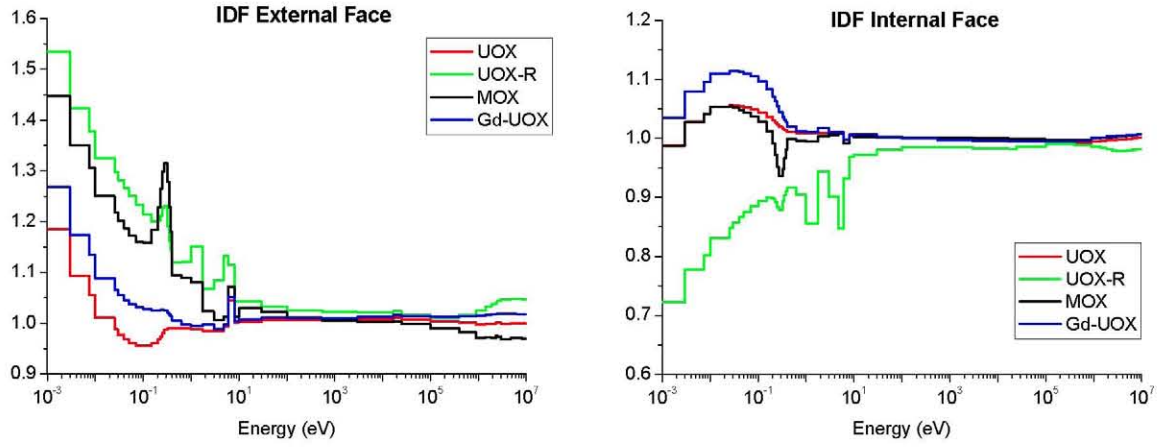

Figure 3. GET Interface Discontinuity Factors in 44 energy-groups for different assembly types.

Different IDF are obtained for the external (north and east faces of nodes in Fig. 1) and internal faces (south and west faces in Fig.1). We decided to study both types of interfaces separately as there are no plans to treat the intranodal effect on the IDF values, so a future neighborhood parameterization will not be able to catch this effect; and also because quarters of assemblies is the most common approach for nodal methods coupled with thermal-hydraulics nowadays.

Regarding the MOX fuel assembly, the computed modal jumps are represented in Fig. 4 as a function of the eigenmode. In 44 energy-groups, 44 modes are obtained which can be real or complex. Consequently, modal jumps are also real or complex, and if complex, there are pairs of complex conjugate values. A stronger correction is again found for the external interfaces, as it was observed for the IDF in the physical space.

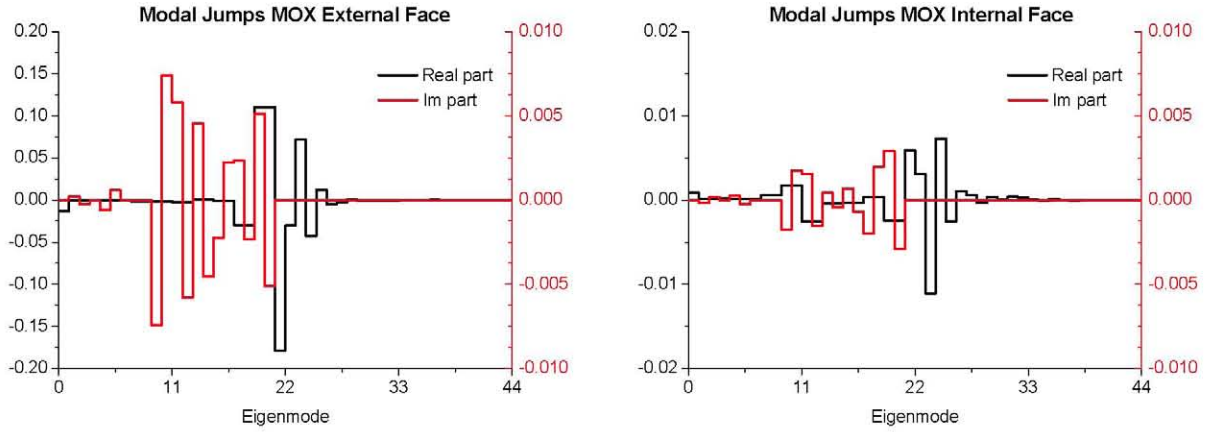

Figure 4. Modal jumps for the MOX fuel assembly in 44 energy-groups.

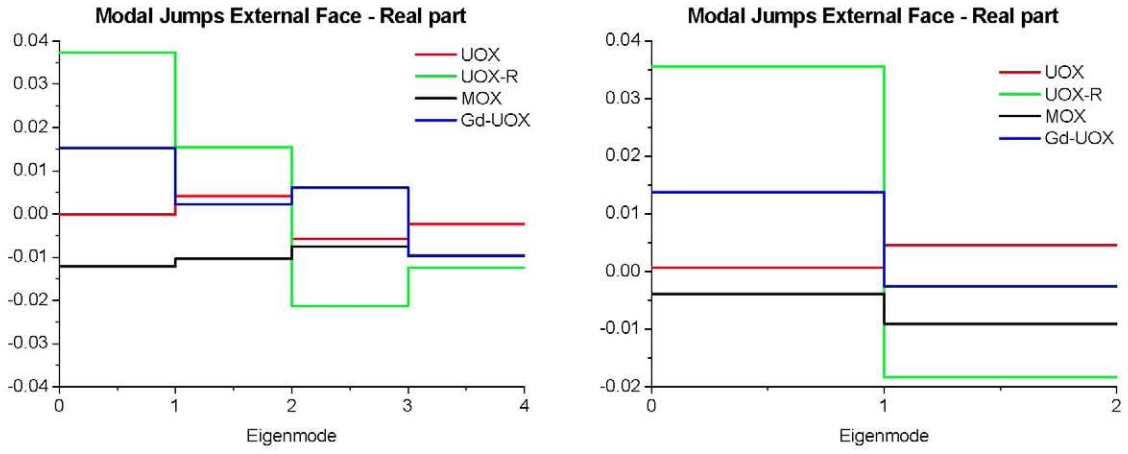

Figure 5. Modal jumps for the four types of fuel assemblies in 4 and 2 energy-groups.

Fig. 5 shows the modal jumps computed in 2 and 4 energy groups for all the fuel assembly types. Only the real part is shown, since the imaginary part is zero in those group structures for all the

assembly types. As in the physical space, the type of heterogeneity inside the assemblies affect the fundamental and transitory modes in different ways.

4.2. Color-set Calculations

When the assembly is surrounded by other types of assemblies, the neutron flux distribution differs significantly from the one calculated in infinite medium, and then, discontinuity factors and modal jumps vary appreciably from the ones calculated in infinite medium. Fig. 6 shows the IDF computed for the external face of the MOX assembly when its environment is perturbed according to the 1D and 2D color-set configurations shown in Fig. 2. The values obtained for the Single Fuel Assembly (FA) are also included. The computed MJ are shown in Fig. 7, where only the real part of the complex values is represented.

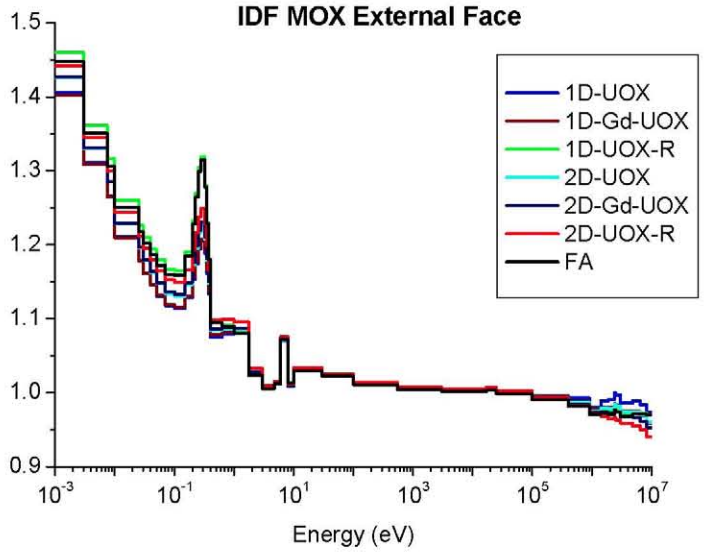

Figure 6. GET Interface Discontinuity Factors in 44 energy-groups for the external face of the MOX fuel assembly in different 1D and 2D color-set configurations.

The IDF are mostly affected on the thermal energy range with neighborhood, although for few energy groups all of them are notably affected. Regarding the modal jumps, the perturbation of the values is concentrated on the middle range transient modes, where the modes are ordered by increasing value of the eigenvalue real part.

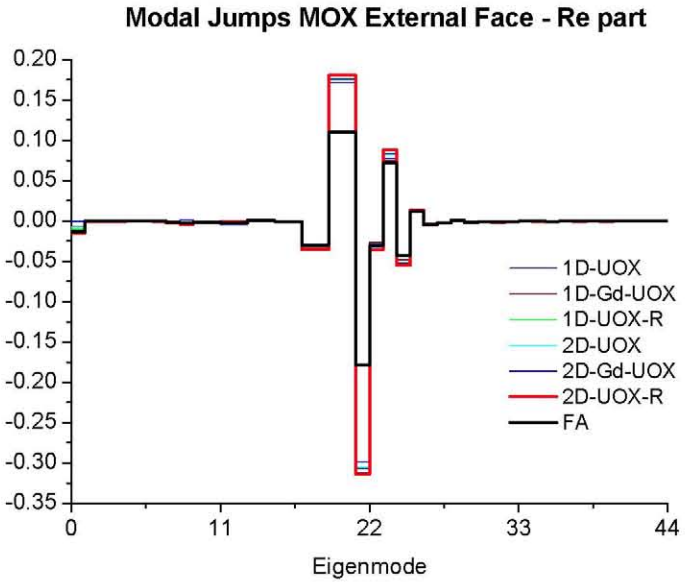

Figure 7. Real part of the modal jumps in 44 energy-groups for the external face of the MOX fuel assembly in different 1D and 2D color-set configurations.

4.3. Testing the implementation in COBAYA3

To assess whether modal jumps are adequate and useful to correct diffusion calculations, a cluster of four quarters of the different fuel assembly types shown if Fig. 1 was chosen: the uranium-oxide fresh fuel assembly (UOX), the depleted UOX fuel assembly with control rods (UOX-R), the UOX assembly with Gd pins (Gd-UOX) and the mixed-oxide fuel assembly (MOX) (see Fig. 8).

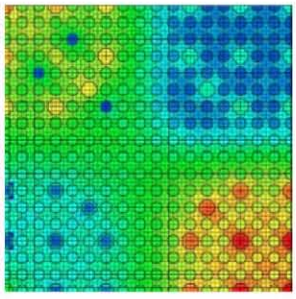

Figure 8. Cluster of four types of 17x17 fuel assemblies.

First, a NEWT transport calculation (reference) was performed and exact nodal macroscopic cross-sections and interface discontinuity factors and modal jumps were obtained. Then, the following nodal diffusion calculations were performed with COBAYA3 code in 2, 4, 8 and 44 energy groups:

a. Using both exact macroscopic cross sections and IDF or MJ from the reference calculation. The expected error in this case is zero, and the purpose of this calculation is to provide a way to verify the correctness of the implementation.
b. Using exact macroscopic cross sections without any type of correction factor. The obtained errors are due to the use of the standard homogenization approximation and the lower order method employed.
c. Using exact macroscopic cross sections and IDF computed in a single assembly calculation with different correction values for the external and internal interfaces.
d. Using exact macroscopic cross sections and MJ computed in a single assembly calculation with different correction values for the external and internal interfaces.

In cases c) and d), errors are associated to the use of correction factors from single assembly calculations with zero-current boundary conditions, that differs from the actual conditions for the nodes in the considered cluster configuration.

Comparison of c) and d) provides a way to assess if modal jumps are less influenced by the node environment than IDF, so they will be provide more accurate results when using the values computed in an infinite lattice.

Table I shows the difference in pcm from the reference k-eff and Table II presents the relative power error for all the four cases (a, b, c, d) considered above and computed with COBAYA3.

Table I. Differences in k-eff (pcm) between ANDES and NEWT (reference)

Case	2 groups	4 groups	8 groups	44 groups
a	-18	-18	-18	-18
b	-380	-408	-450	-471
c	-85	-54	-62	-70
d	-88	-22	-44	-76

Table II. Nodal power relative error (%) of ANDES versus NEWT (reference)

Case	2 groups		4 groups		8 groups		44 groups	
a	0.01%	0.03%	0.01%	0.03%	0.01%	0.03%	0.01%	0.03%
	-0.05%	0.00%	-0.05%	0.00%	-0.05%	0.01%	-0.05%	0.01%
b	-0.49%	1.75%	-0.27%	0.80%	-0.35%	0.72%	-0.37%	0.66%
	5.12%	-3.57%	5.81%	-3.22%	5.90%	-3.13%	5.92%	-3.07%
c	0.11%	0.83%	0.48%	-0.20%	0.50%	-0.41%	0.56%	-0.58%
	0.37%	-1.01%	0.61%	-0.49%	0.64%	-0.34%	0.61%	-0.22%
d	-0.41%	1.62%	-0.08%	0.55%	0.07%	0.35%	-0.15%	0.40%
	0.54%	-1.37%	0.73%	-0.84%	0.59%	-0.64%	0.80%	-0.60%

Case a) confirms that diffusion results match transport results almost exactly when using exact equivalent parameters with differences due to numerical errors. In general, it can be seen that the error increases when going from the use of exact correction factors (case a) to single fuel assembly correction factors (cases c and d) and to no correction factors (case b), as it was expected. Comparable results are obtained in all the energy group structures.

If single assembly correction factors are used, errors are similar whether using modal jumps or interface discontinuity factors. The present results do not highlight any important advantage of modal jumps over GET IDF. And configurations where spectral effects are more pronounced than in the considered color-set problems, such as those involving reflector nodes, should be analyzed in the future to test the goodness of modal jumps compared to classical IDF.

5. CONCLUSIONS

An additional form of interface discontinuity factors based on a correction of the modal fluxes instead of the physical fluxes has been presented. In the ACMFD formulation, after diagonalization of the multigroup diffusion matrix, physical fluxes are transformed into modal fluxes in the eigenspace of the diffusion matrix. It is possible then to introduce interface flux discontinuity jumps as the difference of heterogeneous and homogeneous modal fluxes.

When applying the change of base back to the physical space, we find that the heterogeneous physical fluxes are related to the homogeneous ones by an additive term (instead of a multiplicative term as for the classical IDF) which is a matrix-vector product that couples all the modal jumps for each energy group. That matrix is the matrix of eigenvectors which contains information about the spectral response within each material region.

The formulation in the modal space has been implemented in the diffusion code COBAYA3 and assessed by comparison with solutions using classical interface discontinuity factors. It was verified that errors increase when going from the use of exact correction factors to single fuel assembly correction factors and to not using correction factors; and similar errors were found whether using modal jumps or IDF.

On one side configurations where spectral effects are more pronounced than in the considered color-set problems, such as those involving reflector nodes, should be analyzed in the future to test the goodness of modal jumps compared to classical IDF.

On the other side a parameterization study of the MJ and IDF on neighborhood should be performed at the nodal level, to compare the behavior of both formulations in terms of goodness of the fitting and stability of the proposed parameterization.

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